Introduction to the Monte Carlo method

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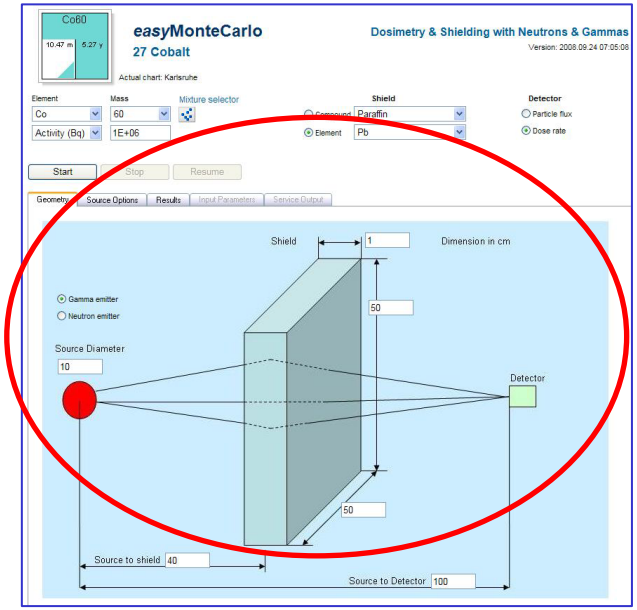
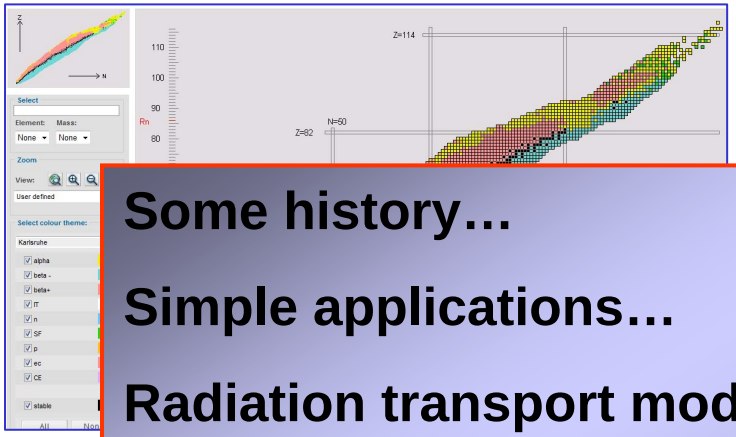
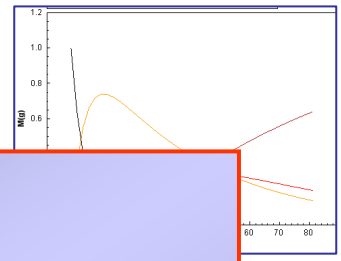
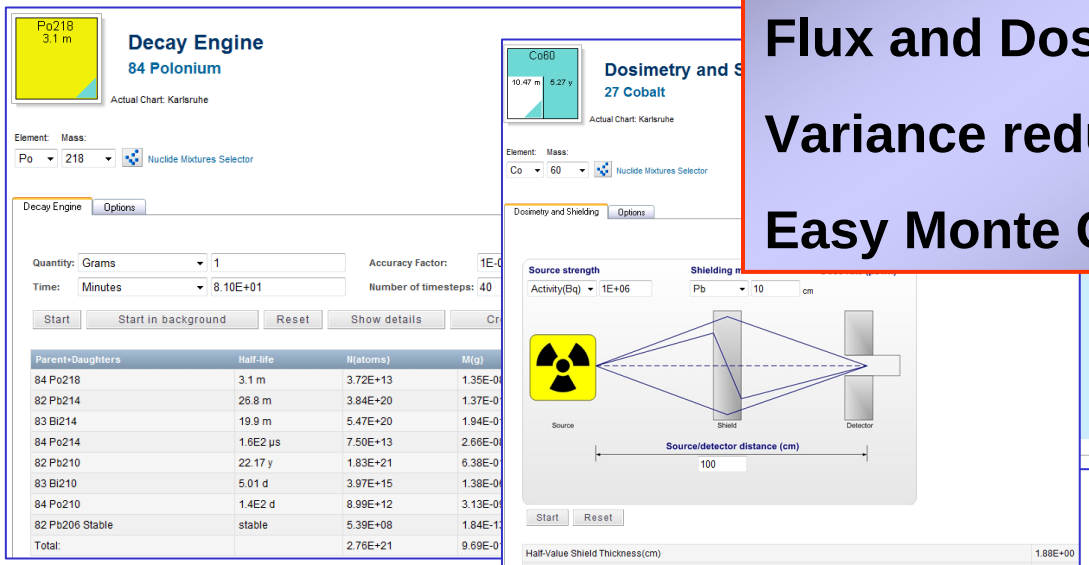
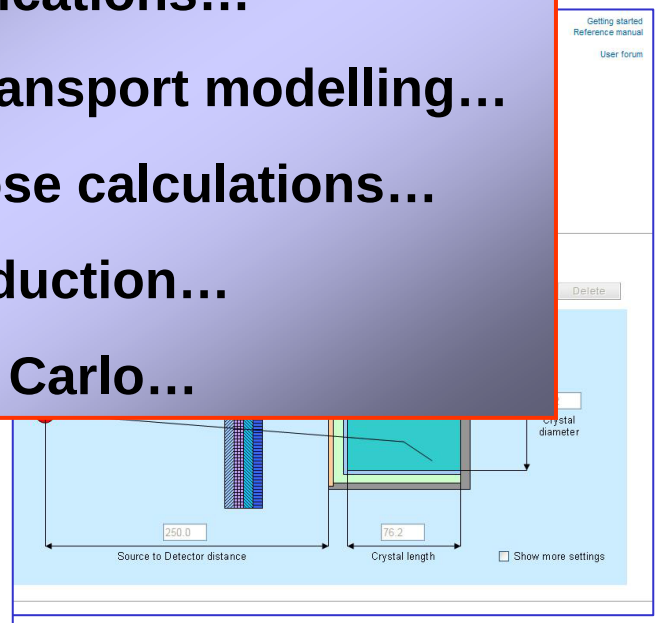










Some history…

Simple applications…

Radiation transport modelling…

Flux and Dose calculations…

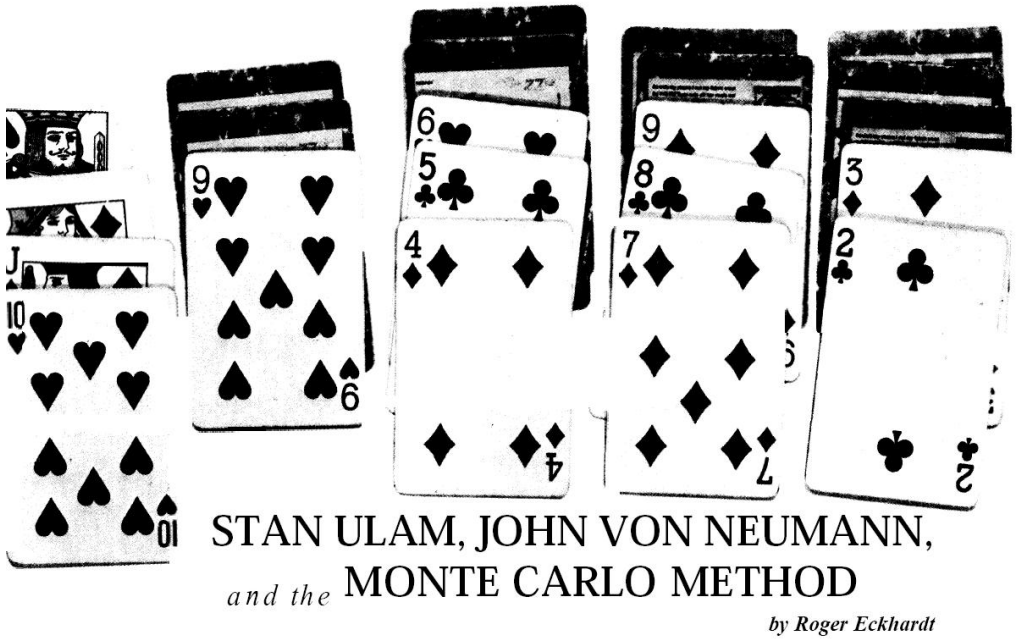
Variance reduction…

Easy Monte Carlo…

Introduction to the Monte Carlo method

Pioneers of the Monte Carlo Simulation Method:

Stanisław Ulam
(1909 –1984)



Stanislaw Ulam is a Polish mathematician who participated in the Manhattan Project and proposed the Teller–Ulam design of thermonuclear weapons. While in Los Alamos, he suggested the Monte Carlo method for evaluating complicated mathematical integrals that arise in the theory of nuclear chain reactions (not knowing that Enrico Fermi and others had used a similar method earlier). This suggestion led to the more systematic development of Monte Carlo by Von Neumann, Metropolis, and others.

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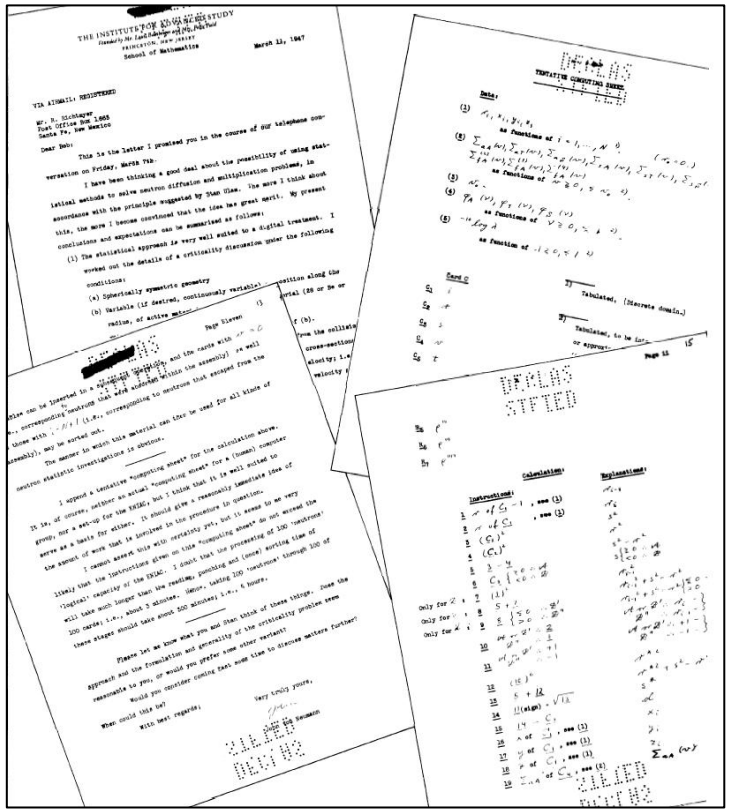
Pioneers of the Monte Carlo Simulation Method:

John von Neumann
(1903 –1957)



Von Neumann was taken by the idea of doing statistical sampling using newly developed electronic computing techniques. The approach seemed to him to be especially suitable for exploring behavior of neutron chain reactions in fission devices. In particular, neutron multiplication rates could be estimated and used to predict the explosive behavior of the various fission weapons then being developed. In March of 1947, he wrote about this to Robert Richtmyer, at that time the Theoretical Division Leader at Los Alamos (see Figure).

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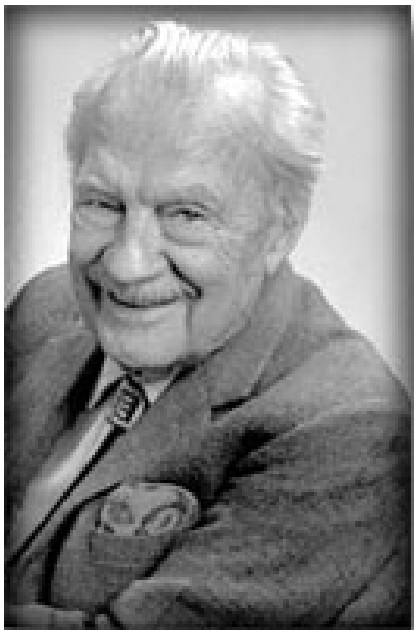
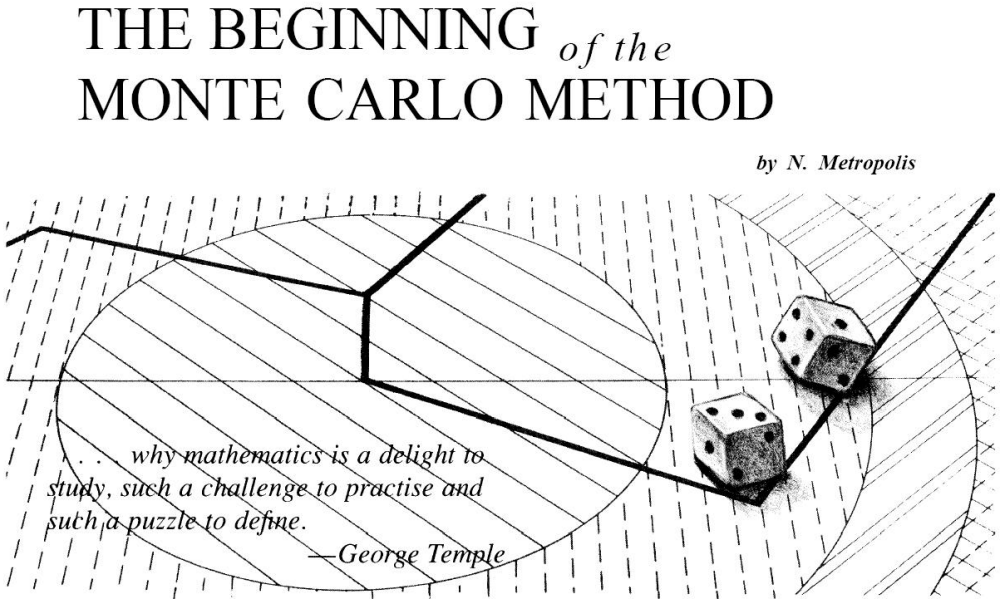
Pioneers of the Monte Carlo Simulation Method:



Nicholas Metropolis (1915-1999)



A team headed by Metropolis carried out the first actual Monte Carlo calculations on the ENIAC computer (the world's first electronic digital computer, built at the University of Pennsylvania) in 1948. The Metropolis algorithm, first described in a 1953 paper by Metropolis, A. Rosenbluth, M. Rosenbluth, A. Teller, and Edward Teller, was cited in *Computing in Science and Engineering* as being among the top 10 algorithms having the "greatest influence on the development and practice of science and engineering in the 20th century."

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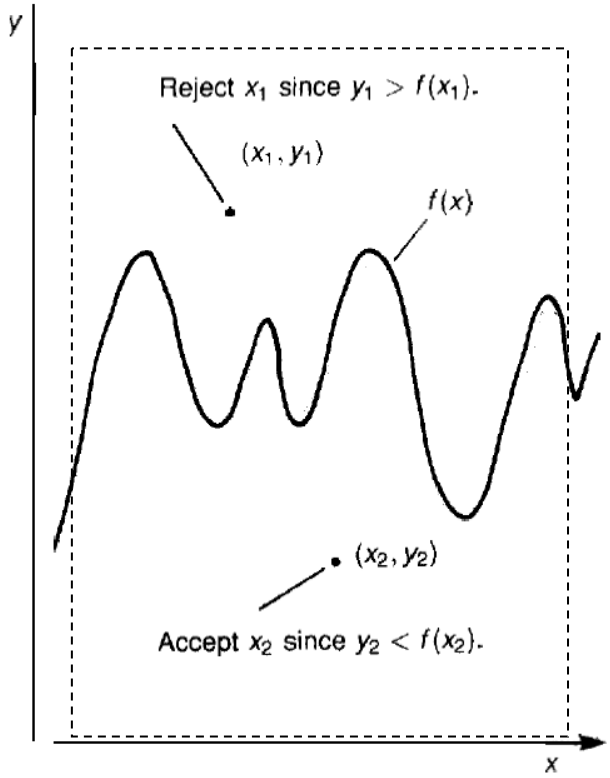
Simple Monte Carlo Application: Function Integration



- If the two numbers x_i and y_i are selected randomly from the range and domain, respectively, of the function f, then each pair of numbers represents a point in the function's coordinate plane (x, y).
- When $y_i > f(x_i)$ the point lies above the curve for $f(x)$, and x_i is rejected; when $y_i \leq f(x_i)$ the points lies on or below the curve, and x_i is accepted.
- Thus, the fraction of the accepted points is equal to the fraction of the area below the curve.

This technique, first proposed by John von Neumann, is also known as the acceptance-rejection method of generating random numbers for arbitrary Probability Density Function (PDF).

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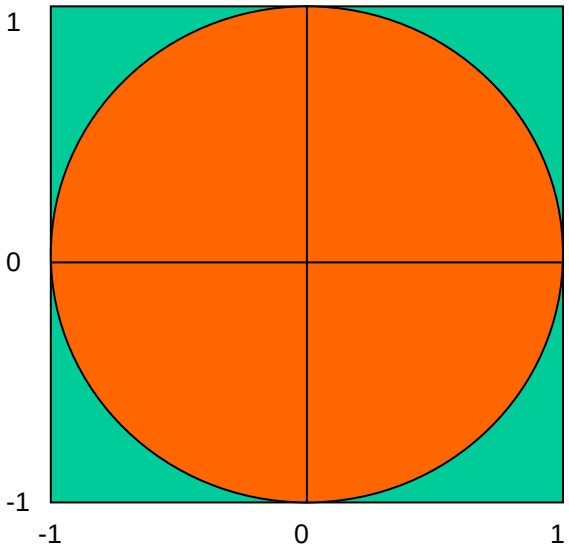
Another Example: Calculation of the π Number

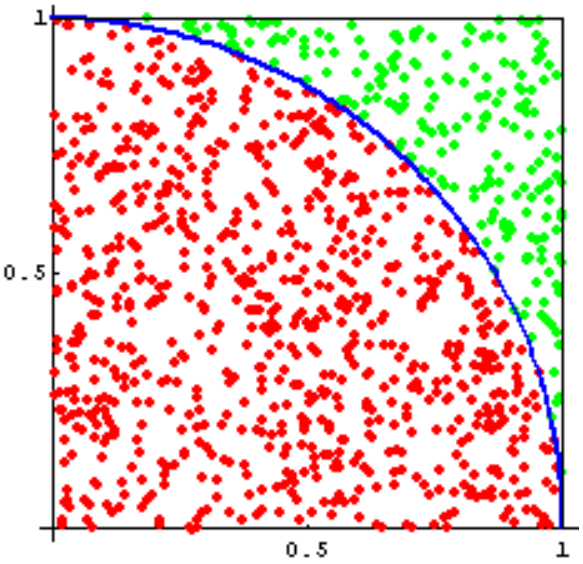


Let us consider a square that encompasses a circle with the radius R = 1. Then,

Area of the square = $2 \times 2 = 4$

Area of the circle = $\pi \times 1^2 = \pi$

$$\frac{Area\ of\ the\ circle}{Area\ of\ the\ square} = \frac{\pi}{4}$$



- A simple Monte Carlo simulation to approximate the value of π could involve randomly selecting of n points (x_i, y_i) in the unit square and determining the ratio $\rho = m / n$, where m is number of points that satisfy $x_i^2 + y_i^2 \leq 1$.

- In a typical simulation of sample size $n = 1000$ there were 787 points satisfying $x_i^2 + y_i^2 \leq 1$, shown in Figure. Using this data, one can obtain

$\rho = 787 / 1000 = 0{,}787$ and $\pi = 4 \cdot 0{,}787 = 3.148$

$\Delta \pi / \pi = m^{-1/2} \approx 3.6\ \%$

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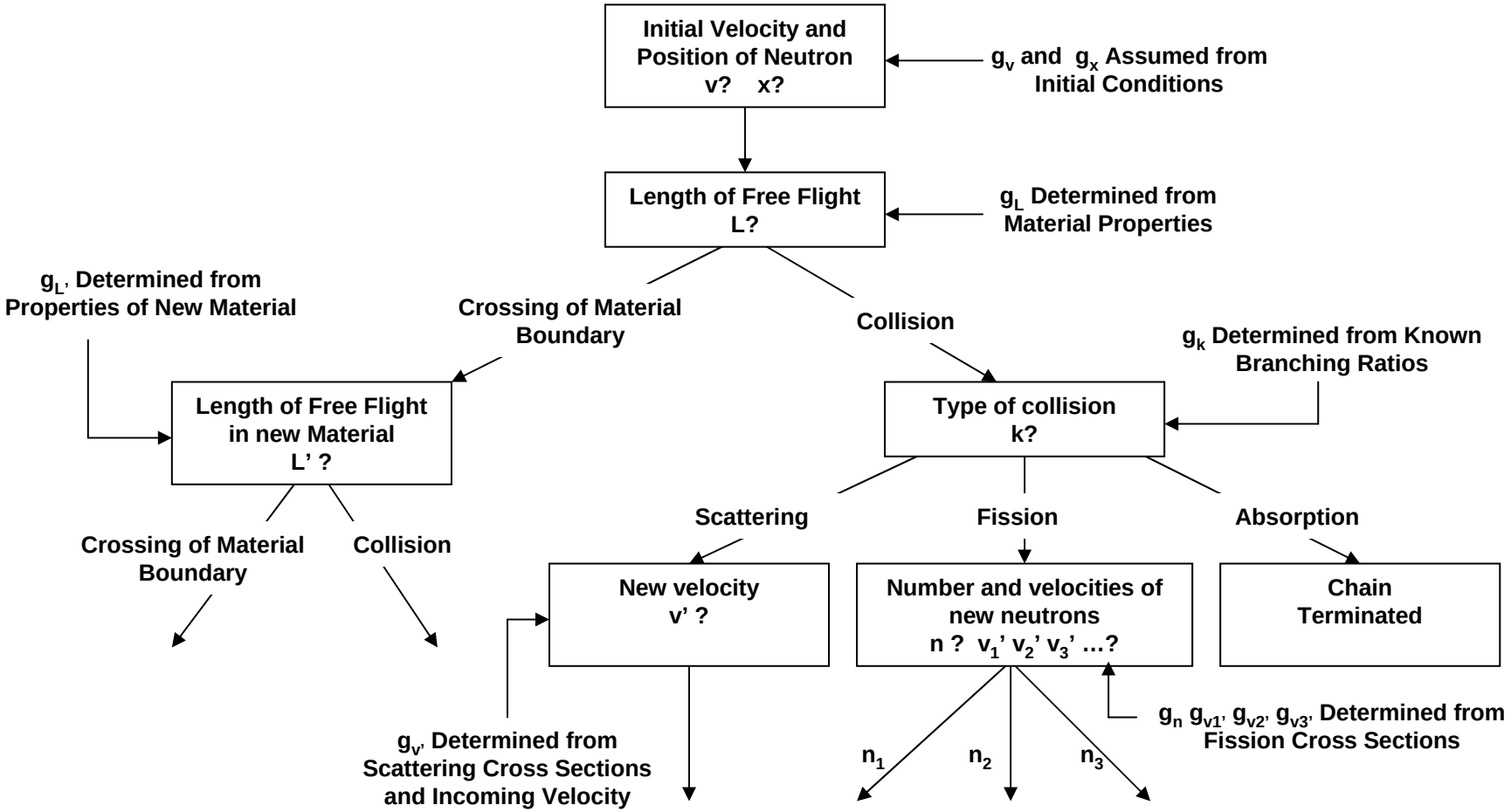
Advanced Application : Neutron Transport

A schematic of some of the decisions that are made to generate the "history" of a neutron in a Monte Carlo calculation.



The non-uniform random-number distribution ***g*** used in the decisions are determined from a variety of nuclear data.

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Sampling Type of the Collision : Photons

Photon interactions :

- Coherent (Rayleigh) scattering
- Incoherent (Compton) scattering
- Photo-effect on K, L_1, L_2 L_3 … atomic shells
- Pair production (nuclear field)
- Triplet production (electron field)
- Photonuclear reactions…

At the given photon energy the contribution of the different interaction processes can be obtained from the energy dependant **photon attenuation coefficients** shown in the Figure to the right.

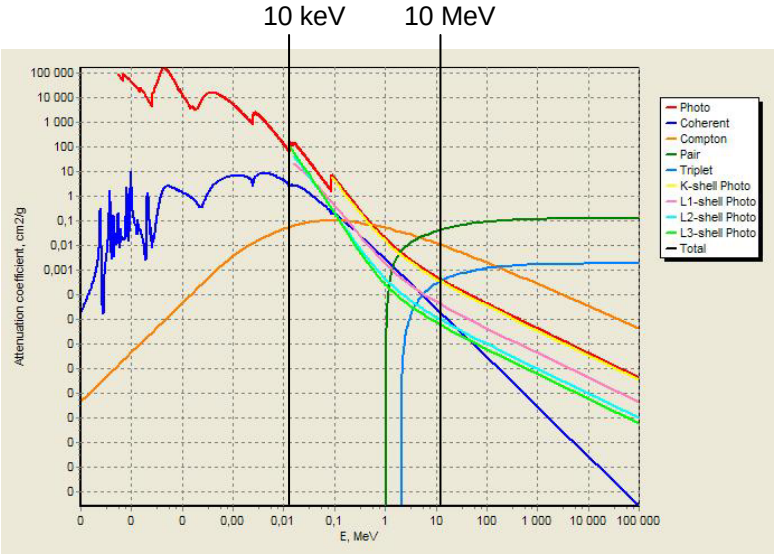


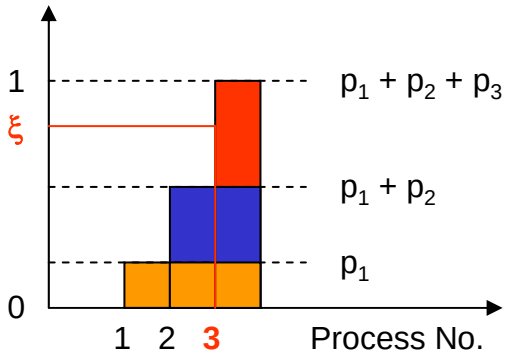
Figure. Photon attenuation coefficients for lead.

Let us consider the 10 keV photon :

Branching ratios (or probabilities) :

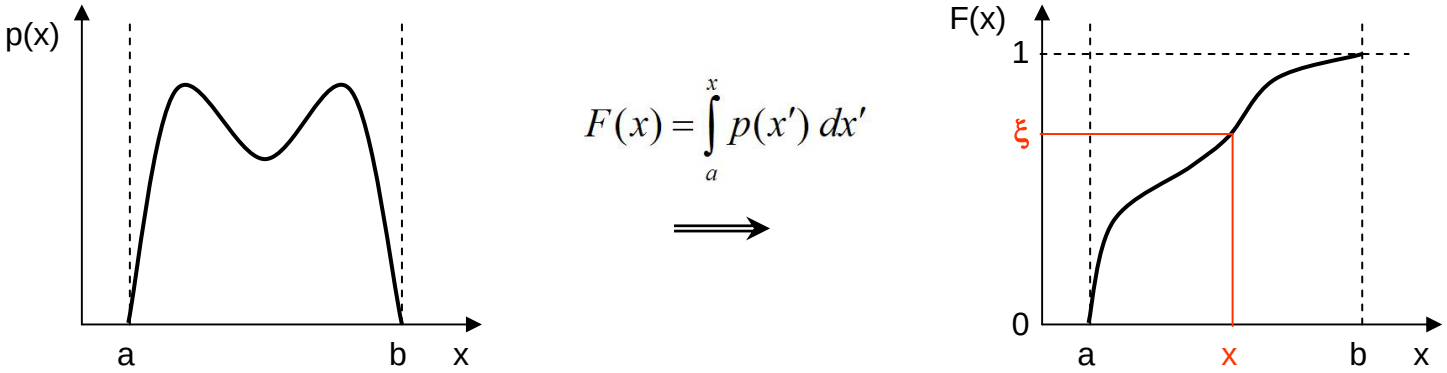
- Process 1: $p_1 = \mu_{Compton} / \mu_{tot}$
- Process 2: $p_2 = \mu_{Rayleigh} / \mu_{tot}$
- Process 3: $p_3 = \mu_{Photo\text{-}effect} / \mu_{tot}$

Let us stack the probabilities to obtain the Probability Distribution Function. Then one can sample the type of the collision (i.e. the process number) using the random number ξ, which is uniformly distributed on [0,1]. See explanation of this algorithms on the graph to the right.



Neutron / Photon Transport : Free Flight / Free Path Simulation

Let us consider the random quantity ***x*** with continuum values from the interval **[a,b]**. If **p(x)** is the respective Probability Density Distribution Function, then, using the analogy with the stacked probabilities from the previous slide, one can obtain the Probability Distribution Function **F(x)** as shown below:



Mathematically the sampling procedure can be expressed using the function $F^{-1}(x)$, the inverse to the Probability Distribution Function F(x):

$$F(x) = \xi \quad \Rightarrow \quad x = F^{-1}(\xi)$$

This is the essence of the **inverse function method**, which was proposed by John von Neumann for generating random values for such random quantities as particle free path, energy and angular distributions etc.

Photon free path simulation using the inverse function method:

$$p(x) = \mu_{tot} \exp(-\mu_{tot} x) \quad \Rightarrow \quad x = -\frac{1}{\mu_{tot}} \ln(\xi)$$

Here ξ is the random quantity with uniform distribution in the interval [0,1].

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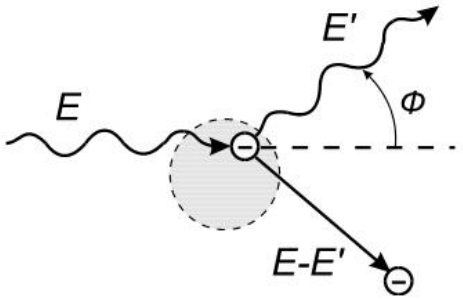
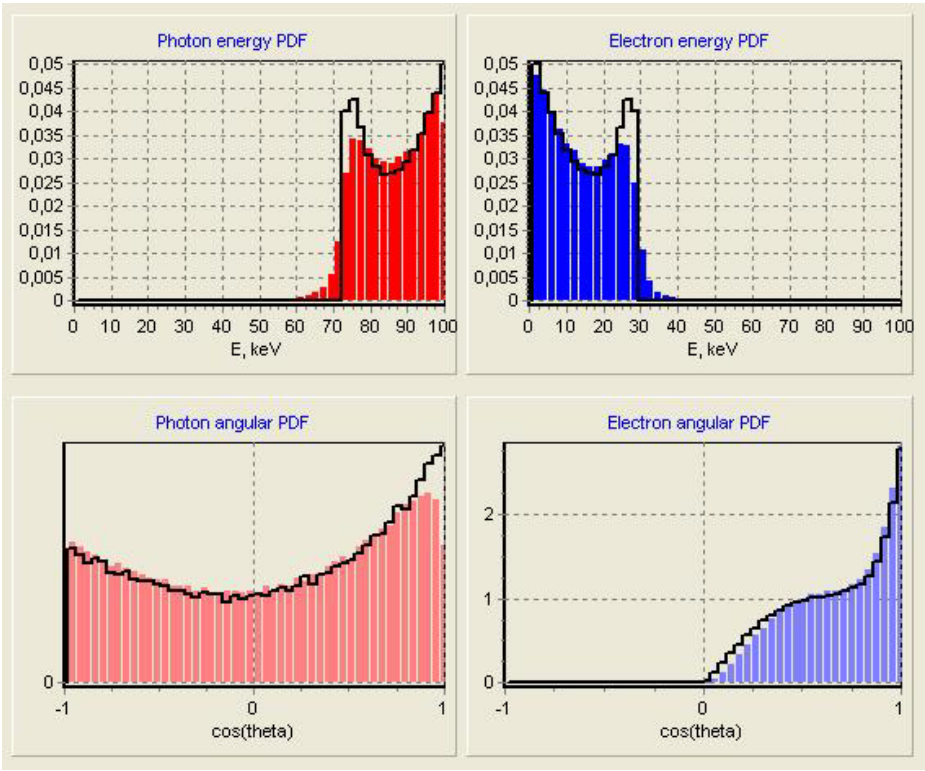
Sampling Photon Collision: Compton scattering

This example shows how the properties of the photon and electron resulting from the Compton scattering can be modeled. The properties are the energy and angular distributions of the new particles – scattered photon and recoil electron.





Click on the graph to see the movie.

Two approaches are shown on the graph (Germanium, 100 keV photons):

- **solid lines** represent sampling technique which is based on the well-known theoretical Klein-Nishina formula for the Compton scattering PDF on free electrons,
- **stacks** show more advanced simulation approach that takes into account atomic electron binding and Doppler broadening effects.

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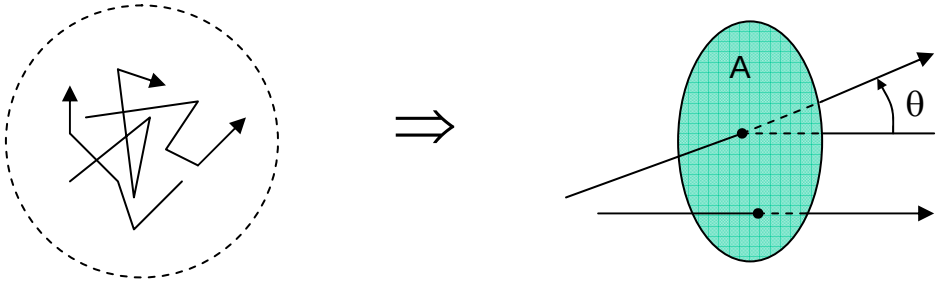
Scoring or Tallying : Two Fundamental Tallies

N - total number of tracks sampled

M - number of tracks, which crossed surface A



$\mu = \cos\theta$

➢ **Particle Current:** The number of particles crossing surface A normalized per one source particle

$$J = \frac{\sum_{i=1}^{M} 1}{N} = \frac{M}{N} \qquad [J] = 1$$

➢ **Particle Flux:** The number of particles crossing surface A normalized per one source particle and per square centimeter of the surface area seen from the direction of the particle. This area is calculated as $A_\mu = A\,|\mu|$, where μ is the absolute value of cosine of angle between surface normal and particle trajectory.

$$\Phi = \frac{\sum_{i=1}^{M} 1/|\mu_i|}{NA} \qquad [\Phi] = cm^{-2}$$

Note: The particle current and particle flux can be expressed using the conventional units, i.e. $[J] = s^{-1}$ and $[\Phi] = cm^{-2}s^{-1}$, by multiplying them by the source strength (number of particles emitted per second).

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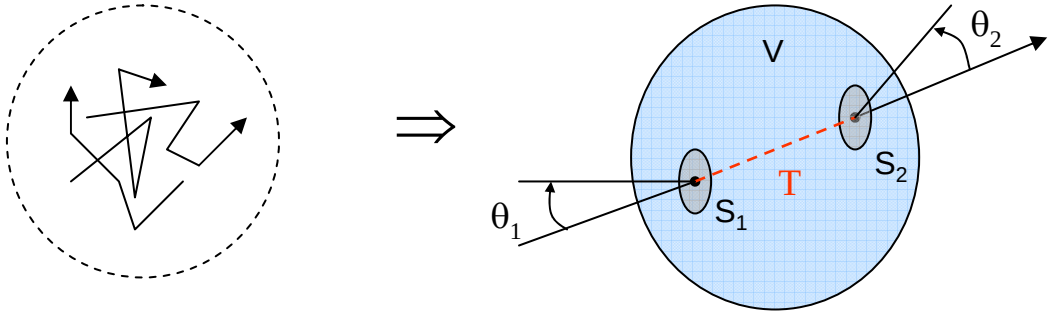
Cell Particle Flux: Track-Length Estimator

The particle flux definition on the previous slide gives the value of the flux averaged over a surface, so called the **Surface Flux Tally**. If we are interested in the particle flux averaged over a cell, then the **Track-Length Tally** will be more suitable.

N - total number of tracks sampled

M - number of tracks, which crossed cell V



The estimate of the particle flux averaged over cell is given by the following formula:

$$\Phi = \frac{\sum_{i=1}^{M} T_i}{N V}$$

Where, T is the track length of particles inside the cell, and V is the cell volume.

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Tallying Gamma / Neutron Dose Rates

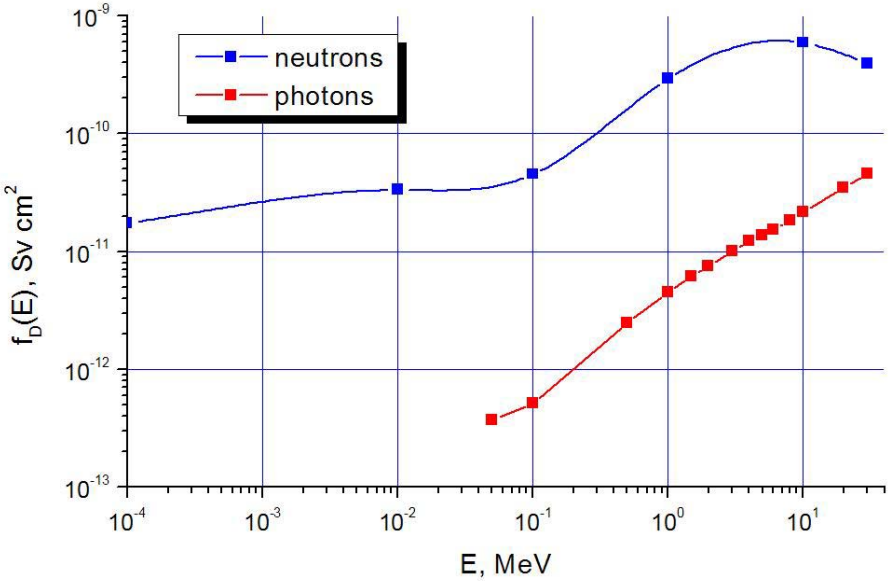
The Gamma / Neutron Dose Rate (Sv/h) can be presented as the linear functional from the photon flux energy distribution $\Phi(E)$ ($MeV^{-1}cm^{-2}s^{-1}$) in the point of interest:

$$\dot{D} = \int_0^{+\infty} \Phi(E) \cdot f_D(E) \cdot dE$$

Here $f_D(E)$ is energy dependent "photon-flux-to-dose-rate" conversion function, which depends on

- the radiation type and energy of particles,
- the properties of absorbing medium (air, water, tissue etc.),
- the dose value of interest (KERMA, absorbed, equivalent, ambient or effective dose).

Thus, to calculate the dose rate, one needs to score the product of a flux estimate (e.g., given by the surface or cell flux tally) with an appropriate value of the corresponding "photon-flux-to-dose-rate" conversion function.



M. Pelliccioni, Overview of Fluence-to-Effective Dose and Fluence-to-Ambient Dose Equivalent Conversion Coefficients for High Energy Radiation Calculated Using Fluka Code, Radiation Protection Dosimetry, 88(4) (2000) 279–297.

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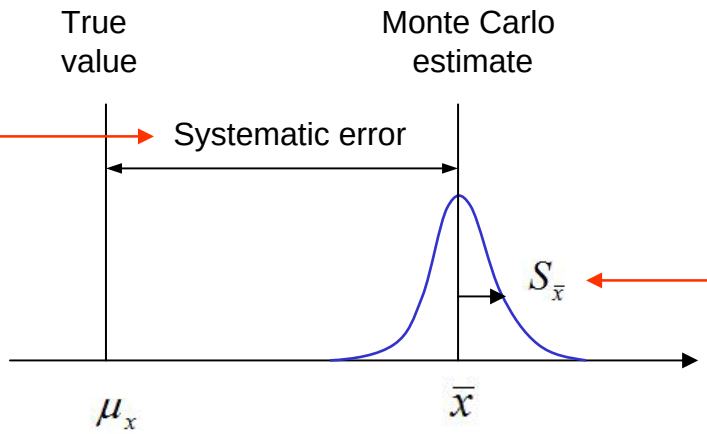
Accuracy, Precision, Relative Error & Figure of Merit

Accuracy

$$\mu_x - \bar{x}$$

is a measure of how close the expected value <x> is to the true physical quantity μ_x being estimated. The difference between them is called the systematic error, which is seldom known.



Precision

$$S_{\bar{x}} = \sqrt{\frac{\overline{x^2} - \bar{x}^2}{N}} \propto \frac{1}{\sqrt{N}}$$

refers to the uncertainty of the Monte Carlo estimate and not to the accuracy. It is possible to calculate a highly precise result that is far from the physical truth because nature has not been modelled faithfully.

Relative error

is the measure of the calculation (statistical) precision of the Monte Carlo result.

$$R = \frac{S_{\bar{x}}}{\bar{x}} \propto \frac{1}{\sqrt{N}}$$

Guidelines for Interpreting the Relative Error:

Range of R	Quality of the result
0.5 – 1.0	Garbage
0.2 – 0.5	Factor of a few
0.1 – 0.2	Questionable
< 0.1	Generally reliable except for point detector
< 0.05	Generally reliable for point detector

Figure of Merit

$$FOM = \frac{1}{R^2 T} \approx const$$

Here T ~ N is the computer time needed to sample N histories.

FOM serves:

- as the reliability indicator for tally (it must be constant except for small statistical variations),
- as the measure of the efficiency of the Monte Carlo calculation (the higher FOM the better the efficiency), and
- as a useful tool for estimating the time needed to achieve given statistical precision.

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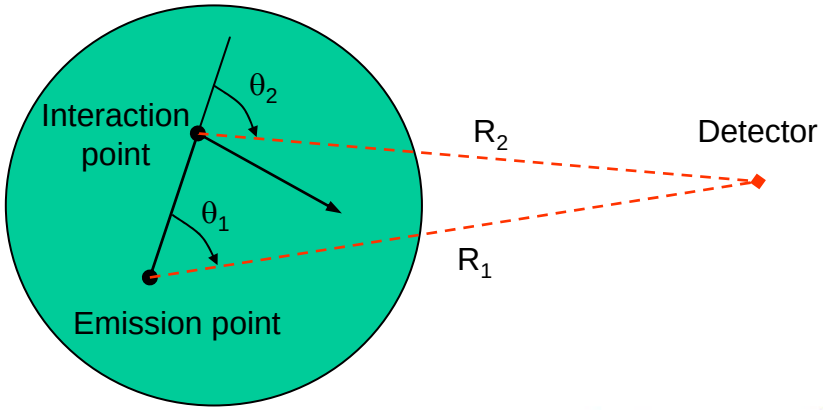
Variance Reduction Example: Point Detector Tally

For very small volumes and heavily shielded sources it can be almost impossible to get either a track-length or surface crossing estimate because of the low probability of crossing into the small volume or because of the very low particle flux outside a heavily shielded object. In such cases the use of the **Point Detector Tally** (one of the **Variance Reduction Techniques**) can provide much greater efficiency (FOM) of the calculation.



$$\Phi = \sum_j p(\mu_j) \frac{e^{-\lambda_j}}{2\pi R_j^2}$$

In the **Point Detector** approach the tally is scored, first, when particles emitted from the source, and, then, after each interaction of primary particles, by calculating the probability for all secondary particles to be emitted or scattered directly to the detector.

The approach therefore is also frequently called as the **Next Event Estimator**.

p(μ) – probability density function for a particle to be emitted / scattered into detector,
μ - cosine of angle between particle trajectory and detector,
R – distance to detector,
λ - total mean free path to detector.

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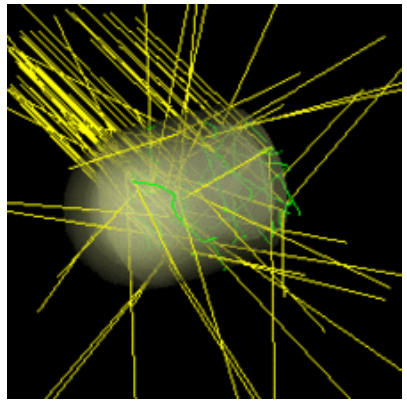
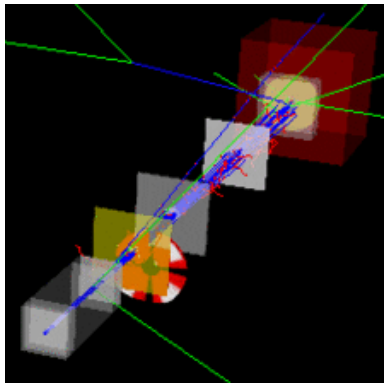
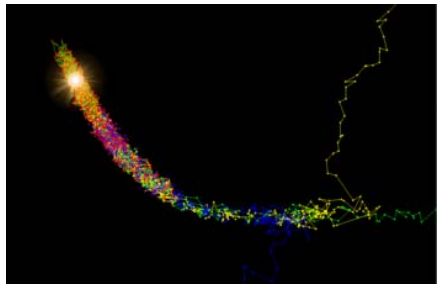
Summary: The primary components of a Monte Carlo simulation method

- *Probability distribution functions (pdf's)* - the physical (or mathematical) system must be described by a set of pdf's.
- *Random number generator* - a source of random numbers uniformly distributed on the unit interval must be available.
- *Sampling rule* - a prescription for sampling from the specified pdf's, assuming the availability of random numbers on the unit interval, must be given.
- *Scoring (or tallying)* - the outcomes must be accumulated into overall tallies or scores for the quantities of interest.
- *Error estimation* - an estimate of the statistical error (variance) as a function of the number of trials and other quantities must be determined.
- *Variance reduction techniques* - methods for reducing the variance in the estimated solution to reduce the computational time for Monte Carlo simulation
- *Parallelization and vectorization* - algorithms to allow Monte Carlo methods to be implemented efficiently on advanced computer architectures.







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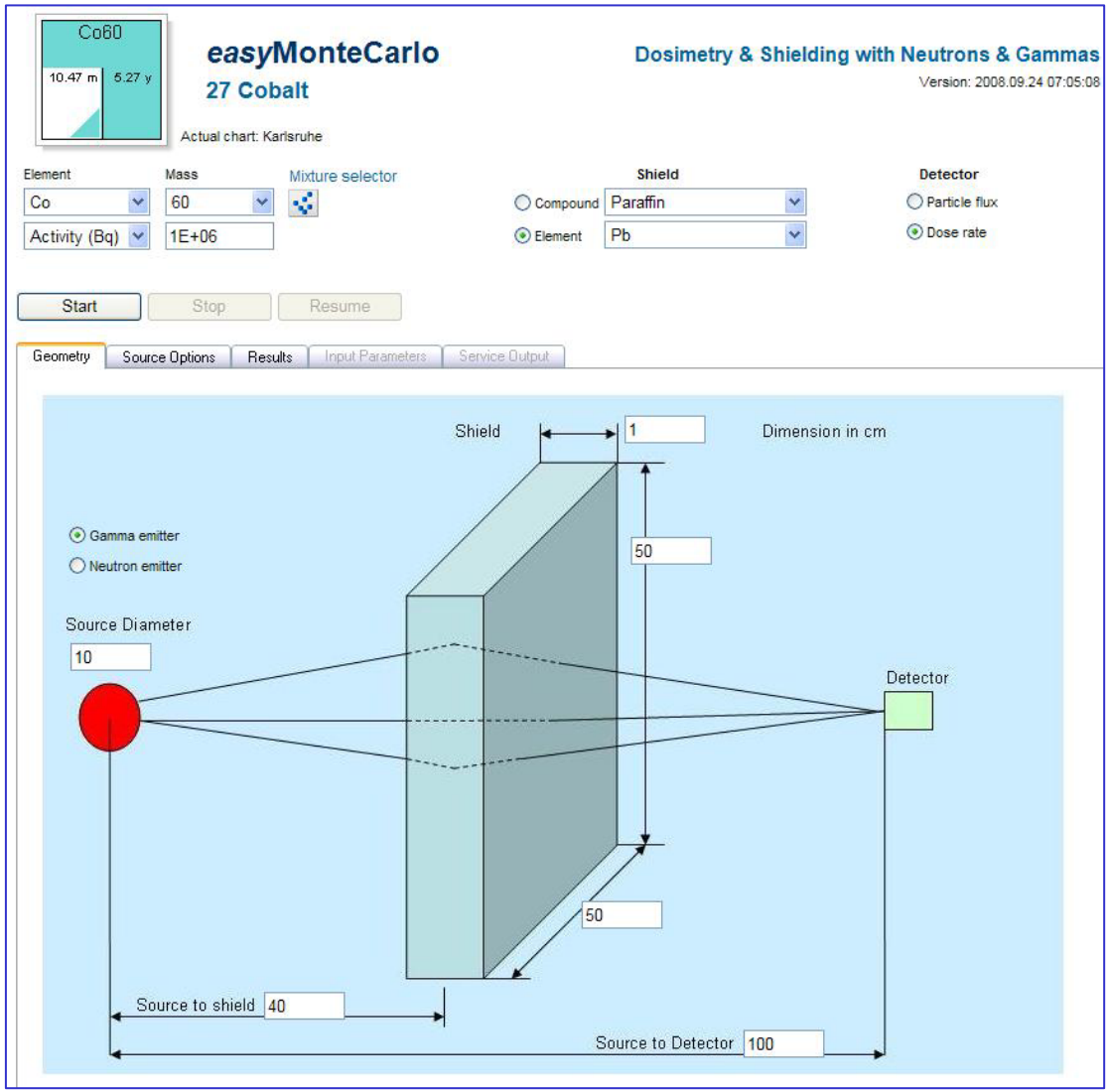
Nucleonica : Easy Monte Carlo for Gamma & Neutron Dosimetry & Shielding Calculations through Web



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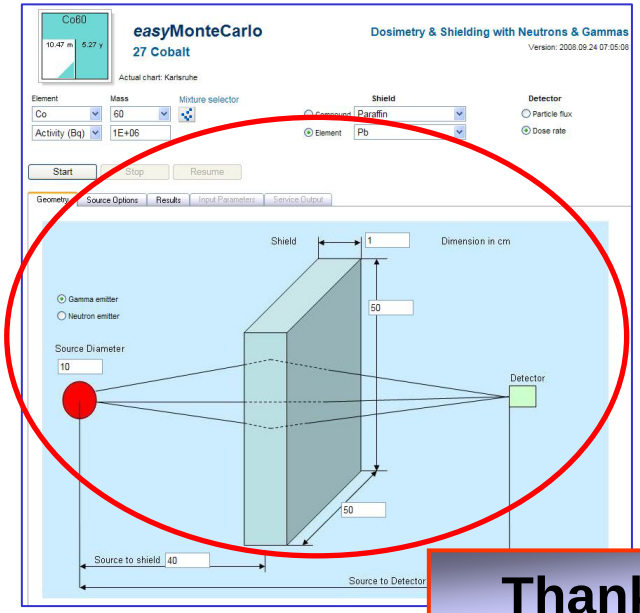

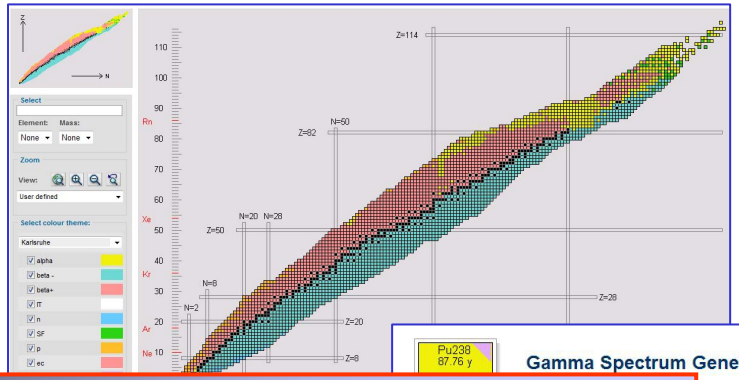

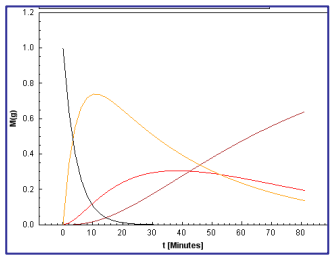

Thank you for your attention…